

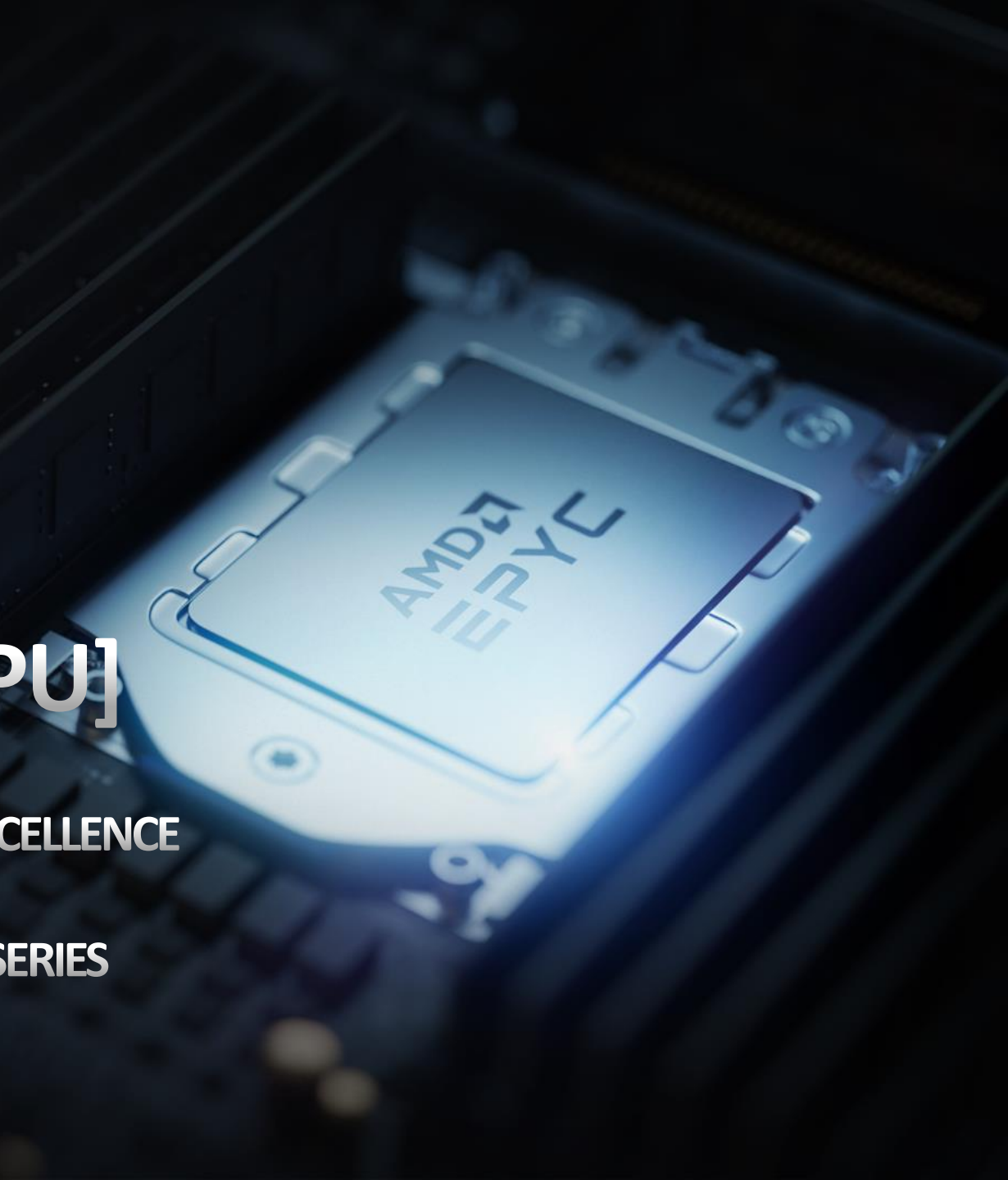


# “WHY AMD FOR HPC” [CPU]

JASON HOGAN-O’NEILL, DIRECTOR HPC CENTRE OF EXCELLENCE

ADVANCED MODELLING AND SIMULATION SEMINAR SERIES

NASA AMES RESEARCH CENTER, JULY 20<sup>TH</sup> 2021



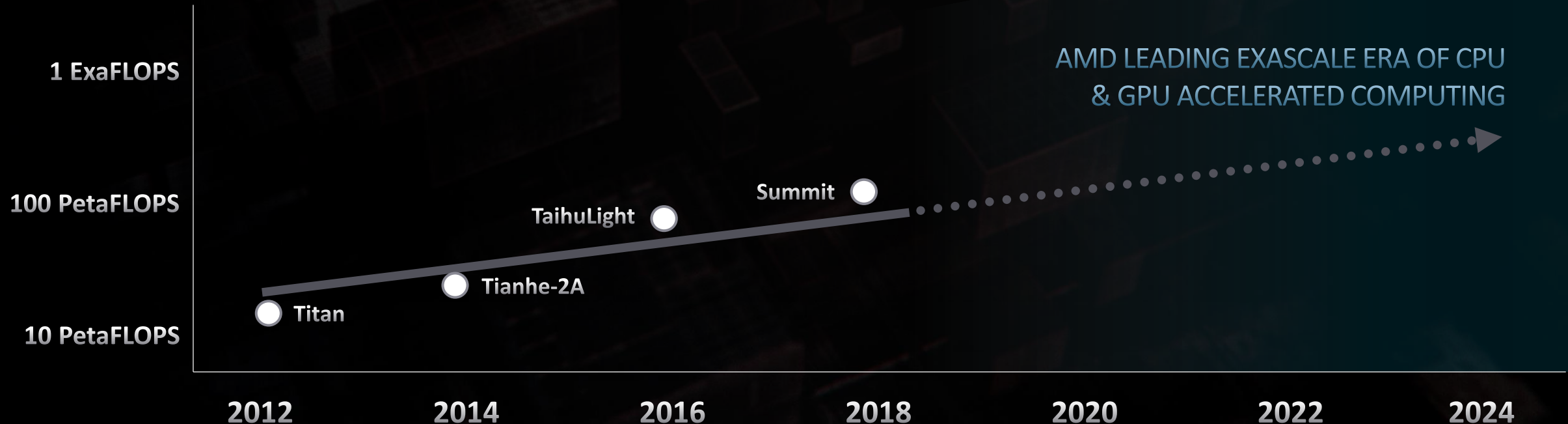
# OVERVIEW

- ❑ **Introduction. Pitch on “Why AMD for CPU”**
- ❑ **SKU orientation**
- ❑ **Architecture**
- ❑ **Software Development Environment**
  - ❑ SPACK HPC Package Management
- ❑ **Applications and their Characterisation**
- ❑ **References**

# ACCELERATED COMPUTING

TACKLING THE WORLD'S MOST IMPORTANT COMPUTATIONAL CHALLENGES

Performance of Top Supercomputers

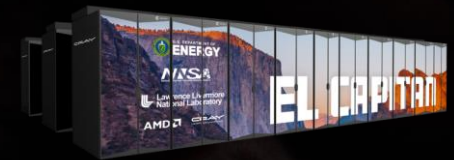
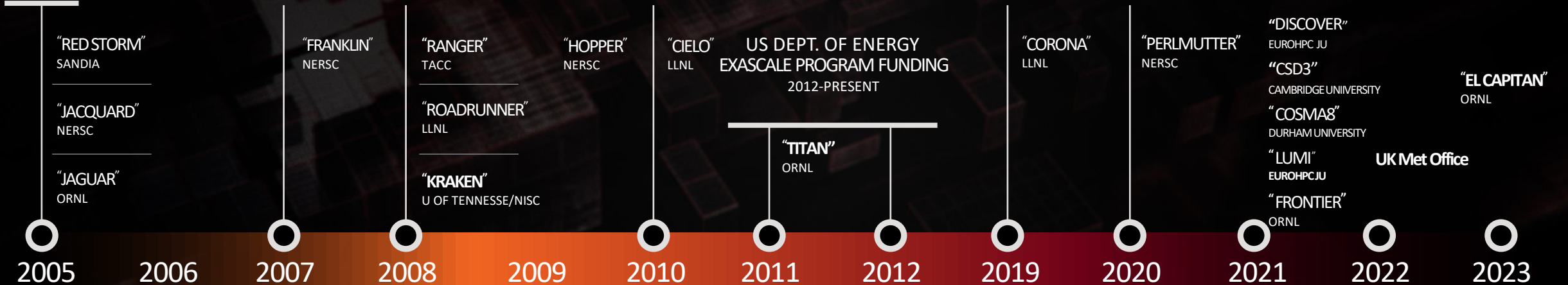


# AMD SUPERCOMPUTING



AMD  
**EPYC**

AMD  
**RADEON**  
INSTINCT



# WHO IS DEPLOYING EPYC?

## BROAD HPC ADOPTION



**SDSC**  
SAN DIEGO SUPERCOMPUTER CENTER



**HLRS**  
High-Performance Computing Center | Stuttgart

  
**METEO  
FRANCE**

*RESEARCH/ACADEMIA*



*COMMERCIAL*

# AMD RELENTLESS TECHNOLOGY INVESTMENT

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**CPU & GPU  
Leadership Roadmaps**

**Leading Edge Process &  
Packaging Technology**

**Next Generation  
Interconnect**

**Accelerated  
Computing**



# CPU ARCHITECTURE ROADMAP



# OPEN SOURCE COMMITMENT TO ENTIRE DEVELOPER STACK

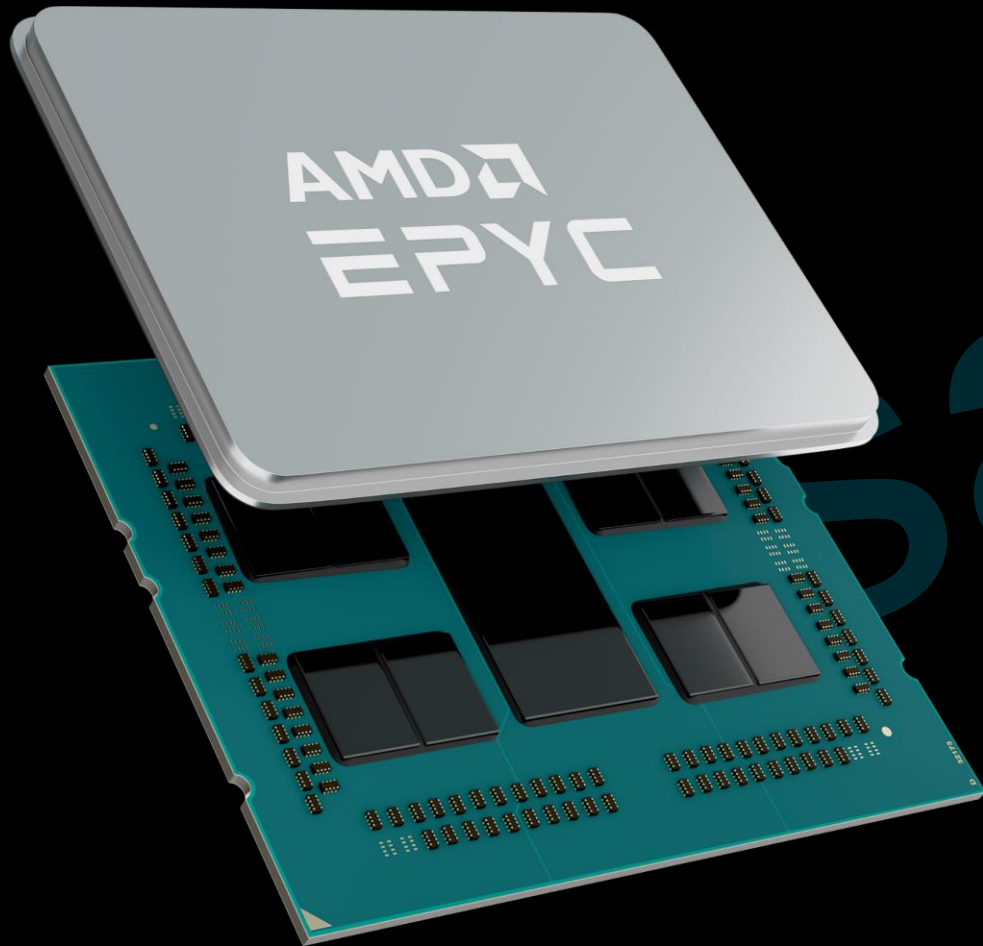
|  | AMD |     |
|--|-----|-----|
|  | CPU | GPU |
| <b>TOOLS</b><br>Profilers, Tracers, and Debuggers<br>for Developers System management for IT | ✓   | ✓   |
| <b>FRAMEWORKS</b><br>Industry leading HPC & ML frameworks for portability                    | ✓   | ✓   |
| <b>LIBRARIES</b><br>Standard Math and Communication Libraries                                | ✓   | ✓   |
| <b>COMPILERS &amp; LANGUAGES</b><br>C/C++, Python, Fortran                                   | ✓   | ✓   |



The image features a dark, high-contrast background of a 3D-rendered microchip. The chip's surface is composed of numerous square and rectangular blocks, some of which are illuminated with a warm, reddish-orange glow, creating a sense of depth and complexity. The AMD logo is centered in the foreground, rendered in a clean, white, sans-serif font. The letters 'A', 'M', and 'D' are in a standard weight, while the final symbol, a stylized triangle, is slightly larger and more prominent.

**AMD**

# KEY FEATURES FOR HPC



Up to **64**  
cores per socket

**“Zen 3”**

**8** Memory  
channels

Up to **256MB**  
L3 cache

**Toolchain**

## **Leadership Compute Throughput**

Best choice for multi-threaded apps and capacity HPC

## **Leadership core performance**

Key for single-threaded apps or to maximize SW investment

## **Consistent leadership since 2017**

Outstanding performance for memory-bound codes

## **Most L3 cache in industry**

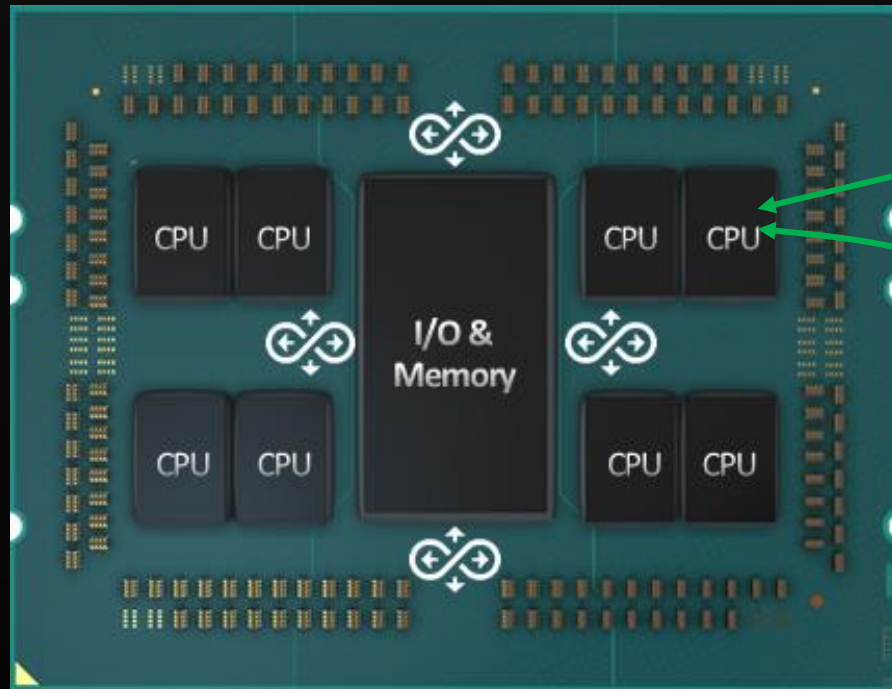
Can enable super-linear scaling of CFD applications

## **Commitment to Open Source**

Prevent vendor lock-in

# “MILAN” BUILDS ON INFINITY ARCHITECTURE

EPYC 7002 & 7003 DIE MCM (8 CCD + 1 IO)



7002 (“Rome”)

|    |    |         |    |    |
|----|----|---------|----|----|
| Z2 | L2 | 16MB L3 | L2 | Z2 |
| Z2 | L2 |         | L2 | Z2 |
| Z2 | L2 | 16MB L3 | L2 | Z2 |
| Z2 | L2 |         | L2 | Z2 |

7003 (“Milan”)

|    |    |             |    |    |
|----|----|-------------|----|----|
| Z3 | L2 | 32 MB<br>L3 | L2 | Z3 |
| Z3 | L2 |             | L2 | Z3 |
| Z3 | L2 |             | L2 | Z3 |
| Z3 | L2 |             | L2 | Z3 |

# AMD EPYC™ PROCESSORS – QUICK COMPARISON

## SOCKET COMPATIBLE COMMON PLATFORM

| CATEGORY               | EPYC 7001              | EPYC 7002                | EPYC 7003                              |
|------------------------|------------------------|--------------------------|--|
| Socket                 | SP3                    | SP3                      | SP3<br>(Not Compatible With Naples MB) |
| Core/Process           | Zen / 14nm             | Zen2 / 7nm               | Zen3 / 7nm                             |
| Max Core Count/Threads | 32/64                  | 64/128                   | 64/128                                 |
| L3 Cache Size          | 64MB                   | 256MB                    | 256MB                                  |
| CCX Arch               | 4 Cores + 8MB          | 4 Cores + 16MB           | 8 Cores + 32MB                         |
| Memory                 | 8 Ch DDR4-2666         | 8 Ch DDR4-3200, NVDIMM-N | 8 Ch DDR4-3200, NVDIMM-N               |
| PCIe Tech & Lane Count | PCIe Gen3, 128L/Socket | PCIe Gen4, 128L/Socket   | PCIe Gen4, 128L/Socket                 |
| Security               | SME, SEV               | SME, SEV                 | SME, SEV, SNP                          |
| Chipset                | NA                     | NA                       | NA                                     |
| Power                  | 120W - 180             | 120W - 280W              | 120W - 280W                            |

# AMD EPYC™ 7003 CPU ARCHITECTURE

## 7763 CPU - 64 CORE HIGH PERFORMANCE





# AMD EPYC™ 7003 CPU ARCHITECTURE

## 75F3 CPU - 32 CORE HIGH PERFORMANCE / CORE



# AMD EPYC™ 7003 CPU ARCHITECTURE

## 72F3 CPU - 8 CORE HIGH PERFORMANCE / CORE



AMD EPYC™ 7003 SERIES PROCESSOR

MODELS

ALL-IN FEATURE SET

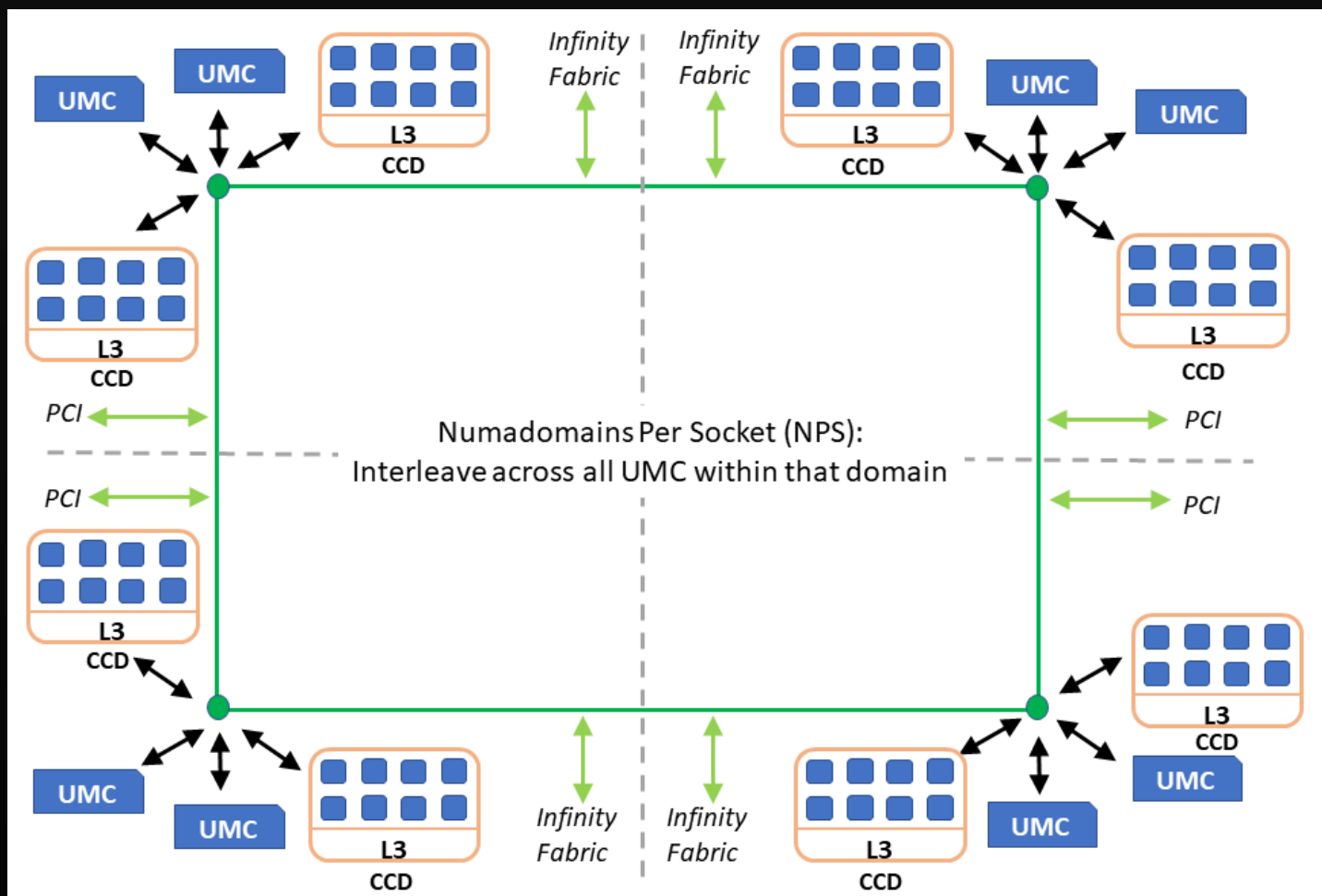
- 8 Channels of DDR4-3200
- 4TB memory capacity
- 128 lanes PCIe® 4
- SMT & Turbo boost
- 18G AMD Infinity Fabric™
- Secure Memory Encryption
- Secure Encrypted Virtualization
- Synchronized fabric and memory clock speeds

| CORES    | AMD<br>EPYC | BASE/BOOST*<br>(up to GHz) | DEFAULT TDP<br>(W) |
|----------|-------------|----------------------------|--------------------|
| 64 CORES | 7763        | 2.45/3.50                  | 280W               |
|          | 7713/P      | 2.00/3.675                 | 225W               |
| 56 CORES | 7663        | 2.00/3.50                  | 240W               |
| 48 CORES | 7643        | 2.30/3.60                  | 225W               |
| 32 CORES | → 75F3      | 2.95/4.00                  | 280W               |
|          | 7543/P      | 2.80/3.70                  | 225W               |
|          | 7513        | 2.60/3.65                  | 200W               |
| 28 CORES | 7453        | 2.75/3.45                  | 225W               |
| 24 CORES | → 74F3      | 3.20/4.00                  | 240W               |
|          | 7443/P      | 2.85/4.00                  | 200W               |
|          | 7413        | 2.65/3.60                  | 180W               |
| 16 CORES | → 73F3      | 3.50/4.00                  | 240W               |
|          | 7343        | 3.20/3.90                  | 190W               |
|          | 7313/P      | 3.00/3.70                  | 155W               |
| 8 CORES  | → 72F3      | 3.70/4.10                  | 180W               |

“F” PERFORMANCE PER CORE OPTIMIZED \*Max boost for AMD EPYC processors is the maximum frequency achievable by any single core on the processor under normal operating conditions for server systems.



# MILAN ARCHITECTURE



UMC = Unified Memory Controller; CCD = Compute Core Die

## COMMENTS:

- More CCDs provide increased memory BW
- PCIe and Infinity fabric assigned per NUMA. Check CTX-6 affinity
- NPS4 shown; NPS2 and NPS1 also possible
- NPS4 provides highest memory bandwidth compared to NPS2 or NPS1
- Data Fabric (DF) Speed has been increased from 1467MHz (Rome) to 1600MHz (Milan)
- 1600MHz is 'coupled' to 3200MHz, i.e. it is exactly 2 cycles in 3200. Extra memory bw increase derives from both increased DF speed and coupled mode.

[jason@milan003 ~]\$ hwloc-ls | less // Shows a snip from hwloc-ls //

```
Group0 L#2
  NUMANode L#2 (P#2 63GB)
    L3 L#4 (32MB)
      L2 L#32 (512KB) + L1d L#32 (32KB) + L1i L#32 (32KB) + Core L#32 + PU L#32 (P#32)
      L2 L#33 (512KB) + L1d L#33 (32KB) + L1i L#33 (32KB) + Core L#33 + PU L#33 (P#33)
      L2 L#34 (512KB) + L1d L#34 (32KB) + L1i L#34 (32KB) + Core L#34 + PU L#34 (P#34)
      L2 L#35 (512KB) + L1d L#35 (32KB) + L1i L#35 (32KB) + Core L#35 + PU L#35 (P#35)
      L2 L#36 (512KB) + L1d L#36 (32KB) + L1i L#36 (32KB) + Core L#36 + PU L#36 (P#36)
      L2 L#37 (512KB) + L1d L#37 (32KB) + L1i L#37 (32KB) + Core L#37 + PU L#37 (P#37)
      L2 L#38 (512KB) + L1d L#38 (32KB) + L1i L#38 (32KB) + Core L#38 + PU L#38 (P#38)
      L2 L#39 (512KB) + L1d L#39 (32KB) + L1i L#39 (32KB) + Core L#39 + PU L#39 (P#39)
    L3 L#5 (32MB)
      L2 L#40 (512KB) + L1d L#40 (32KB) + L1i L#40 (32KB) + Core L#40 + PU L#40 (P#40)
      L2 L#41 (512KB) + L1d L#41 (32KB) + L1i L#41 (32KB) + Core L#41 + PU L#41 (P#41)
      L2 L#42 (512KB) + L1d L#42 (32KB) + L1i L#42 (32KB) + Core L#42 + PU L#42 (P#42)
      L2 L#43 (512KB) + L1d L#43 (32KB) + L1i L#43 (32KB) + Core L#43 + PU L#43 (P#43)
      L2 L#44 (512KB) + L1d L#44 (32KB) + L1i L#44 (32KB) + Core L#44 + PU L#44 (P#44)
      L2 L#45 (512KB) + L1d L#45 (32KB) + L1i L#45 (32KB) + Core L#45 + PU L#45 (P#45)
      L2 L#46 (512KB) + L1d L#46 (32KB) + L1i L#46 (32KB) + Core L#46 + PU L#46 (P#46)
      L2 L#47 (512KB) + L1d L#47 (32KB) + L1i L#47 (32KB) + Core L#47 + PU L#47 (P#47)
  HostBridge
  PCIBridge
    PCI 21:00.0 (InfiniBand)
      Net "ib0"
        OpenFabrics "mlx5_0"
```

Use hwloc-ls to check

- CPU ID affinity per L3
- Location of Mellanox card

All CPU IDs in the shown NUMA domain are logically closest to the network

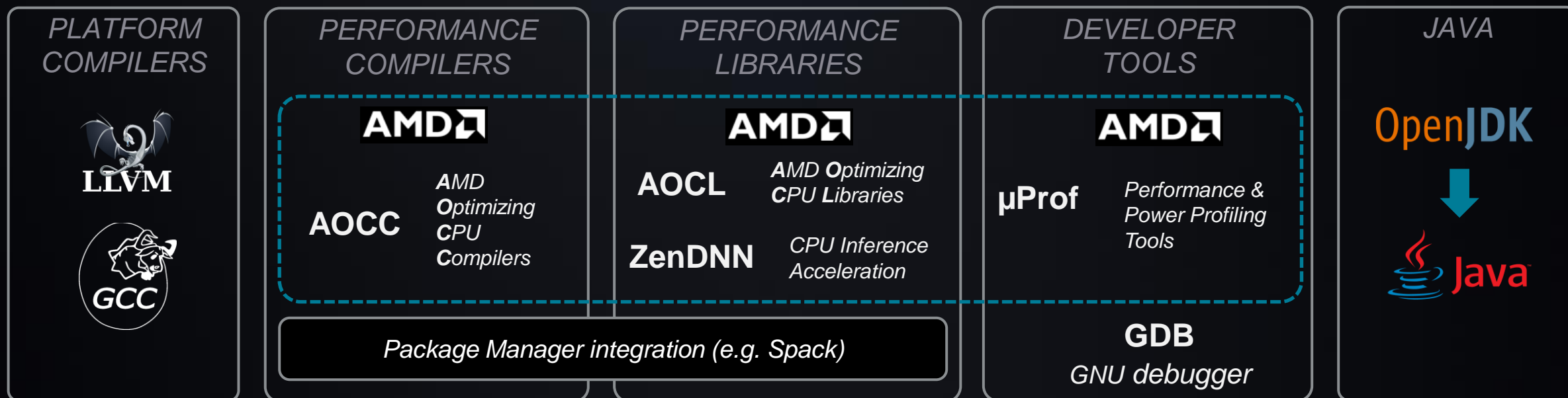
Tip: Use linux command 'seq' to generate lists of CPU IDs for your job, e.g. every second core:

```
[jason@milanLogin ~]$ seq -s , 0 2 127
0,2,4,6,8,10,12,14,16,18,20,22,24,26,28,30,32,34,36,38,40,42,44,46,48,50,52,54,56,58,60,62,64,66,68,70,72,74,76,78,80,82,84,86,88,90,92,94,96,98,100,102,104,106,108,110,112,114,116,118,120,122,124,126
```



# TOOLCHAIN ECOSYSTEM

AMD EPYC SOFTWARE DEVELOPMENT ENVIRONMENT



Use AMD tools for best performance and code efficiency on EPYC CPUs

Compilers → focus on delivering the best out-of-the-box code generation for C, C++, Fortran, Java

Libraries → support common kernels for core math, solvers and FFT

Profiling tools → enable developers to access the full capabilities of EPYC CPUs

*All tools available at [developer.amd.com](https://developer.amd.com)*

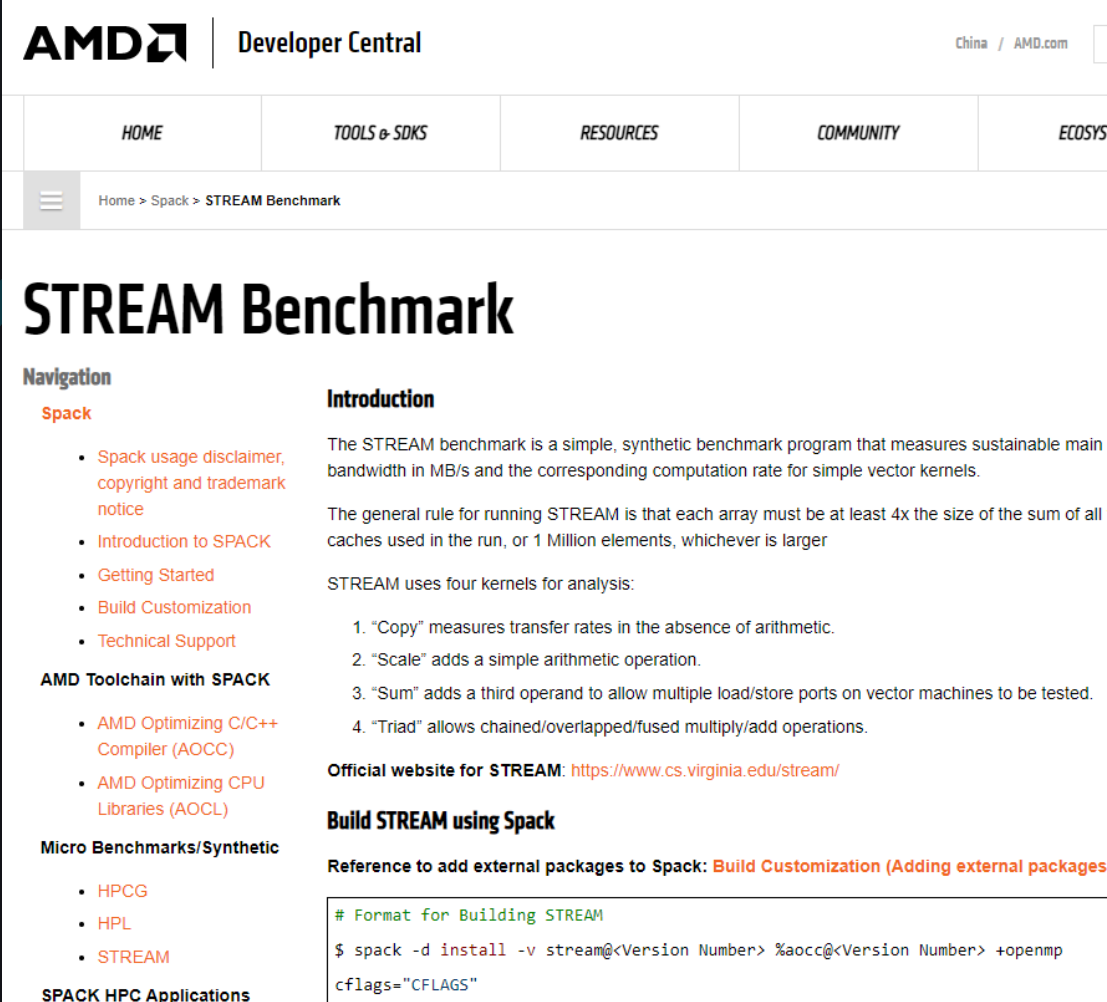
# SPACK: AOCC-OPTIMISED INSTALLATION

Makes it easier for customers and partners to install and test codes and avoid extensive web searches

Install:

- AOCC +AOCL version 3.0 (aligns to “Zen3”)
- Popular synthetics, build and run steps
- Popular HPC Codes, build and run

Go to <https://developer.amd.com/spack/> for application recipes (more being added, e.g. CP2K, Quantum Espresso)



The screenshot shows the AMD Developer Central website. The top navigation bar includes the AMD logo, "Developer Central", and a language selector for "China / AMD.com". Below this is a secondary navigation bar with links for "HOME", "TOOLS & SDKS", "RESOURCES", "COMMUNITY", and "ECOSYS". A breadcrumb trail indicates the current location: "Home > Spack > STREAM Benchmark".

## STREAM Benchmark

**Navigation**

- Spack**
  - Spack usage disclaimer, copyright and trademark notice
  - Introduction to SPACK
  - Getting Started
  - Build Customization
  - Technical Support
- AMD Toolchain with SPACK**
  - AMD Optimizing C/C++ Compiler (AOCC)
  - AMD Optimizing CPU Libraries (AOCL)
- Micro Benchmarks/Synthetic**
  - HPCG
  - HPL
  - STREAM
- SPACK HPC Applications**

**Introduction**

The STREAM benchmark is a simple, synthetic benchmark program that measures sustainable main bandwidth in MB/s and the corresponding computation rate for simple vector kernels.

The general rule for running STREAM is that each array must be at least 4x the size of the sum of all caches used in the run, or 1 Million elements, whichever is larger

STREAM uses four kernels for analysis:

1. "Copy" measures transfer rates in the absence of arithmetic.
2. "Scale" adds a simple arithmetic operation.
3. "Sum" adds a third operand to allow multiple load/store ports on vector machines to be tested.
4. "Triad" allows chained/overlapped/fused multiply/add operations.

**Official website for STREAM:** <https://www.cs.virginia.edu/stream/>

**Build STREAM using Spack**

Reference to add external packages to Spack: [Build Customization \(Adding external packages\)](#)

```
# Format for Building STREAM
$ spack -d install -v stream@<Version Number> %aocc@<Version Number> +openmp
cflags="CFLAGS"
```

# SPACK: AOCC-OPTIMISED INSTALLATION

## AOCL:

```
[jason@MilanLogin ~]$ spack list amd
```

```
==> 8 packages.
```

```
amdblis  amdfftw  amdlibflame  amdlibm  amdscalapack  bamdst  llvm-amdgpu  namd
```

## AOCC Compiler:

```
[jason@MilanLogin ~]$ spack list aocc
```

```
==> 1 packages.
```

```
aocc
```

## # Example: Build Optimized Stream Binary

```
spack install stream %aocc@2.3.0 +openmp cflags="-O3 -mcmmodel=large -DSTREAM_TYPE=double \
-mavx2 -DSTREAM_ARRAY_SIZE=2500000000 -DNTIMES=10 -ffp-contract=fast -fnt-store"
```

```
spack load stream
```



# AMD EPYC™ CPUS: APPLICATIONS

# APPLICATION DOMAINS

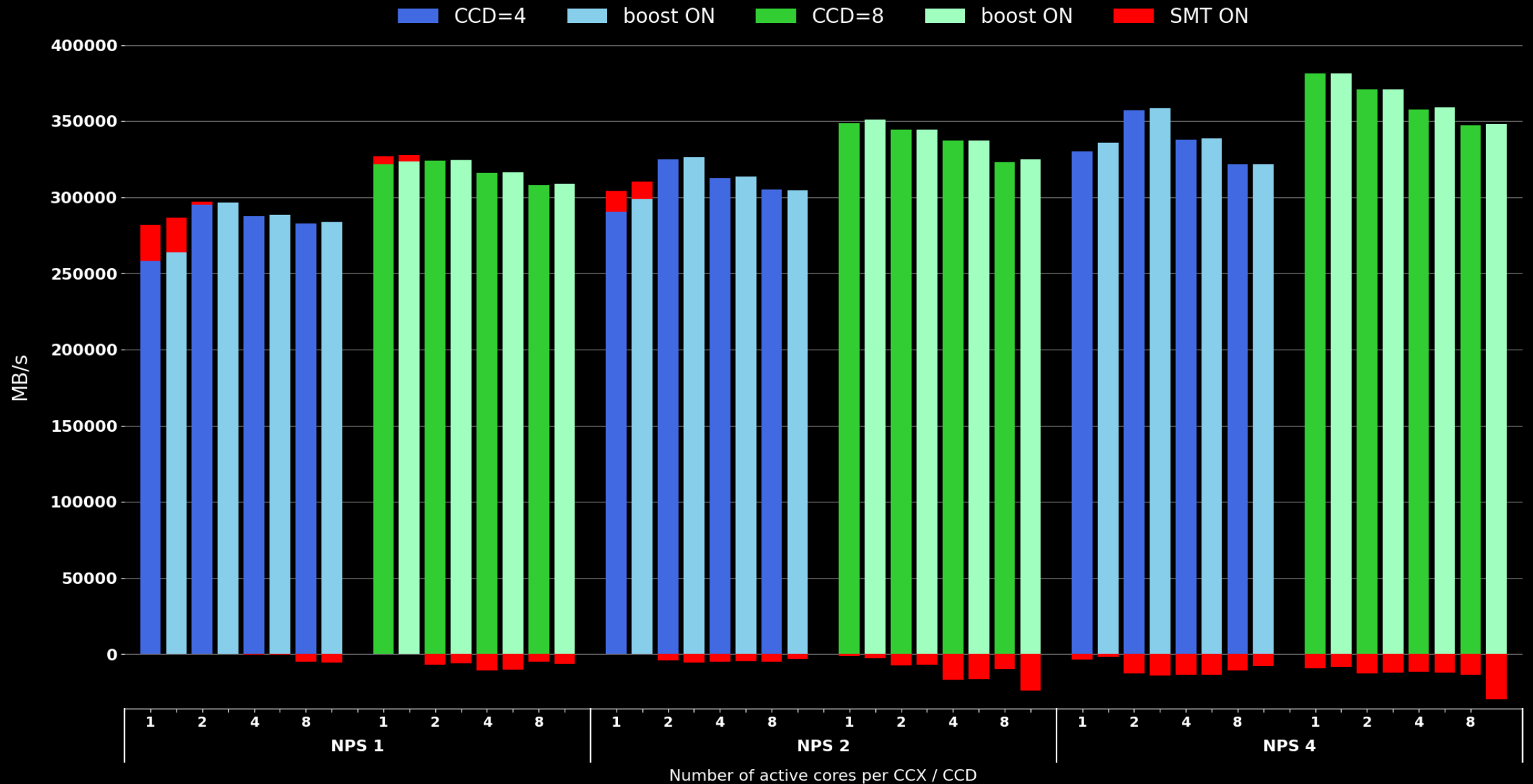
The following domains are where AMD typically performs well in HPC.

VERY STRONG coverage across all real workloads (Life Sciences investigation starting 21Q2)

| Sector                          | Problem Set   | Example Code Set (not exhaustive)  |
|---------------------------------|---|--|
| Automotive                      | <ul style="list-style-type: none"><li>➤ Computational Fluid Dynamics (CFD)</li><li>➤ Structural Codes ('Finite Element Analysis' - FEA)</li></ul> | <ul style="list-style-type: none"><li>➤ StarCCM+, OpenFOAM, ...</li><li>➤ LSDYNA, NASTRAN, ABAQUS, ...</li></ul> |
| Aerospace                       | Same problem set as Automotive  | Same code set as Automotive  |
| Oil and Gas                     | <ul style="list-style-type: none"><li>➤ Reservoir</li><li>➤ Seismic</li></ul>   | Often rely on ISV codes. Some have their own inhouse solvers   |
| Weather                         | Weather Forecast and Climate Modelling  | WRF, UFS, GFS, Unified Model, ...  |
| HPC Centers, including Academia | Wide range of codes: Molecular Dynamics, Quantum Chemistry, weather, CFD, inhouse codes   | GROMACS, NAMD, CP2K, LAMMPS, VASP, WRF, OpenFOAM, inhouse, ...   |
| Government Labs                 | Security conscious (SME?); all problem sets above may apply   | Any of the above + inhouse codes   |

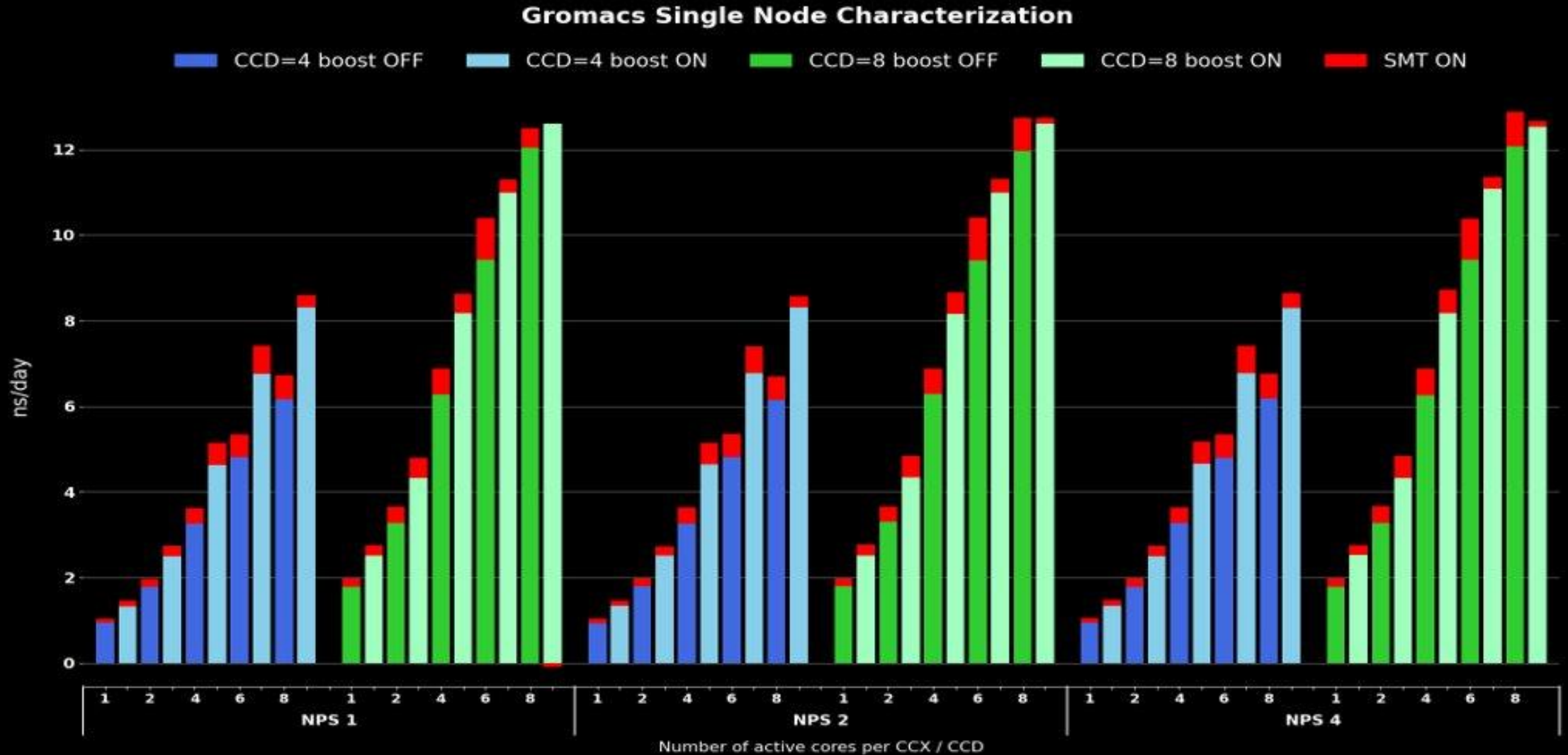


# Stream Single Node Characterization



**Higher is Better**

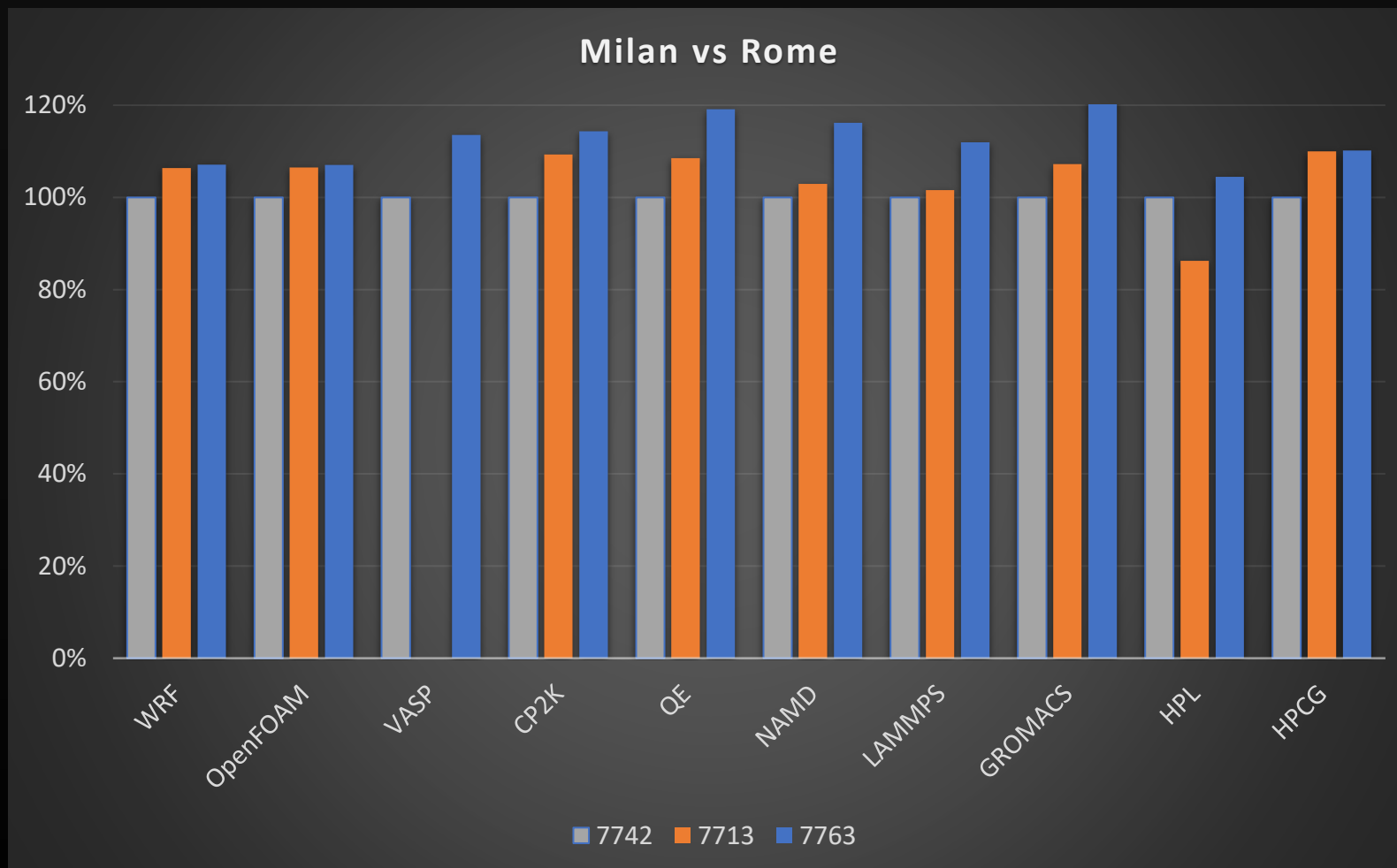
# GROMACS – water\_1536



**Higher is Better**

# 2<sup>ND</sup> GEN EPYC™ VS 3<sup>RD</sup> GEN EPYC™: COMPARING 64 CORES

Compare 7742 v 7713 v 7763



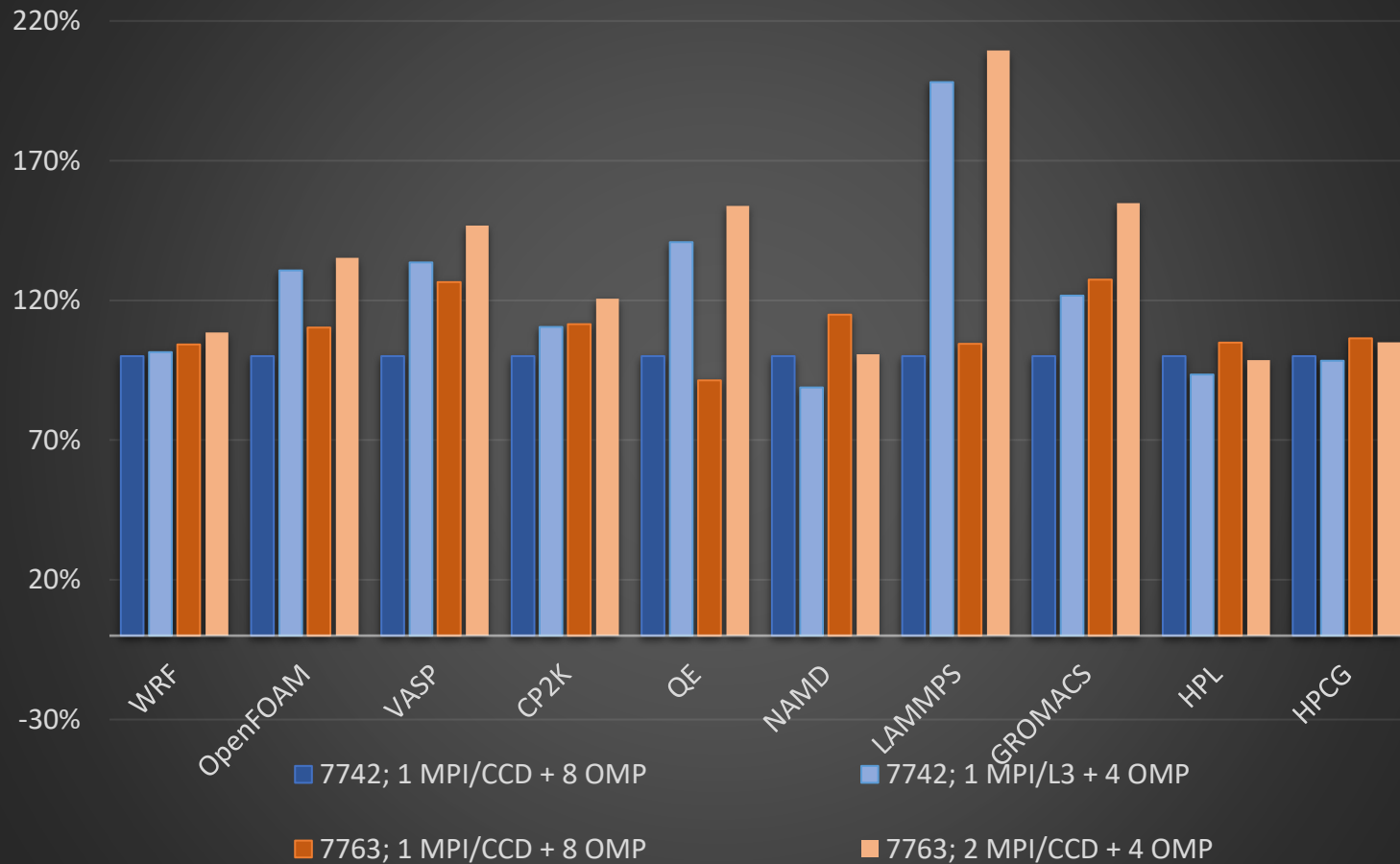
|          | 7713 | 7763 |
|----------|------|------|
| WRF      | 6%   | 7%   |
| openFOAM | 7%   | 7%   |
| VASP     | -    | 14%  |
| CP2K     | 9%   | 14%  |
| QE       | 9%   | 19%  |
| NAMD     | 3%   | 16%  |
| LAMMPS   | 2%   | 12%  |
| GROMACS  | 7%   | 22%  |
| HPL      | -14% | 4%   |
| HPCG     | 10%  | 10%  |

*Relative to 7742*

**Higher is Better, Rome 7742 = 100%**

# BENEFITS OF 3<sup>RD</sup> GEN EPYC™ OVER 2<sup>ND</sup> GEN EPYC™

MPI+OpenMP Milan vs Rome



Compare relative performance between 2<sup>nd</sup> Gen EPYC 7742 and 3<sup>rd</sup> Gen EPYC 7763 with all cores active per CCD but with differing MPI + OMP layout<sup>Δ</sup>:

- 7742: 1 MPI / CCD x 8 OMP \*
- 7742: 1 MPI / L3 x 4 OMP
- 7763: 1 MPI / CCD x 8 OMP
- 7763: 2 MPI / CCD x 4 OMP

→ Milan improves on Rome

\*Normalise to '1' and compare

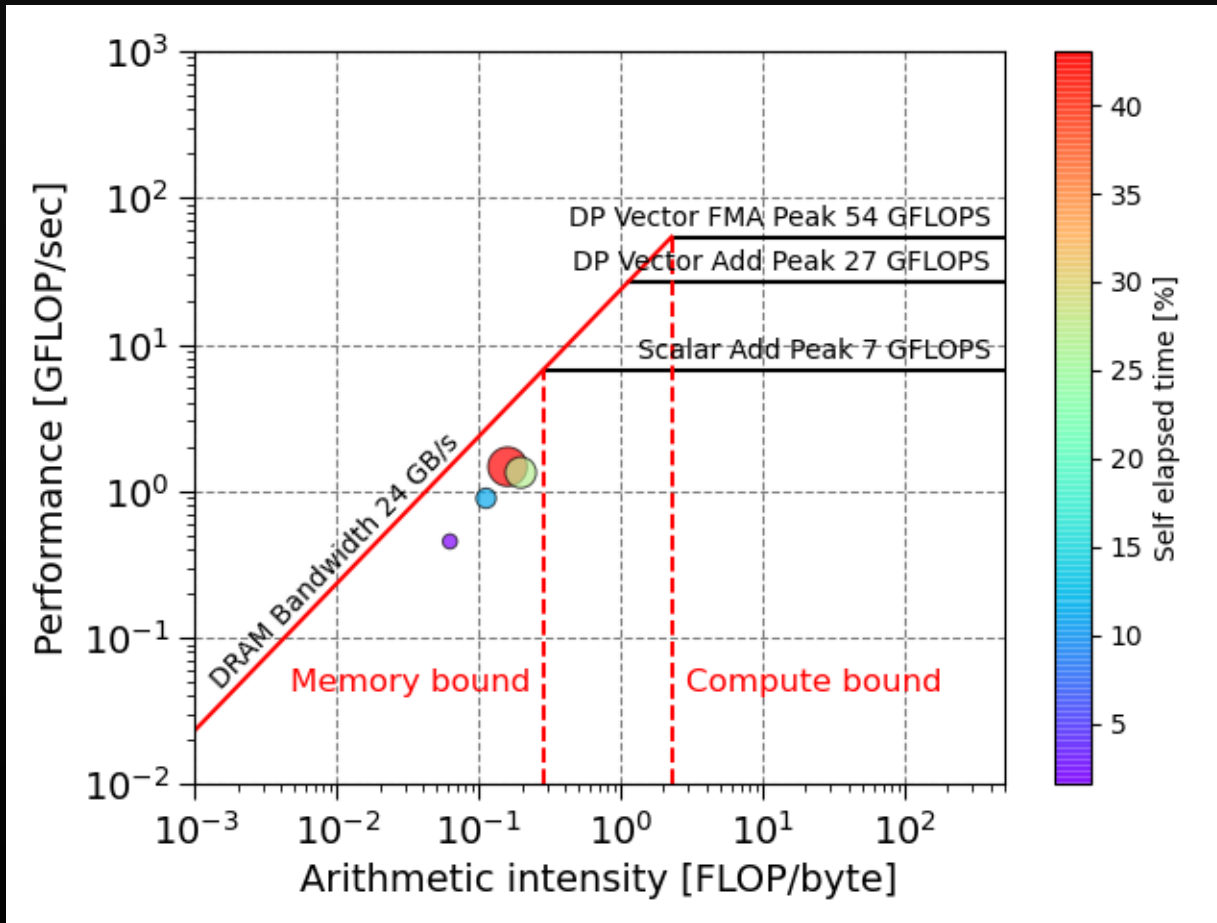
Δ OpenFOAM and VASP are MPI only

|    |    |      |    |    |
|----|----|------|----|----|
| Z2 | L2 | 16MB | L2 | Z2 |
| Z2 | L2 | L3   | L2 | Z2 |
| Z2 | L2 | 16MB | L2 | Z2 |
| Z2 | L2 | L3   | L2 | Z2 |

|    |    |          |    |    |
|----|----|----------|----|----|
| Z3 | L2 | 32 MB L3 | L2 | Z3 |
| Z3 | L2 |          | L2 | Z3 |
| Z3 | L2 |          | L2 | Z3 |
| Z3 | L2 |          | L2 | Z3 |

# MEMORY BANDWIDTH v CLOCK FREQ

LAMMPS, EMA



2 competing system-level choke-points:

- Bandwidth to main memory
- 'Compute Bound' ('frequency')

These are mutually exclusive to each other

Perform roofline analysis to confirm where hot-routine lands (red circle)

We have performed this analysis on a number of popular HPC codes across CFD, Weather, Quantum Chemistry, Molecular Dynamics: Codes are memory bound or borderline

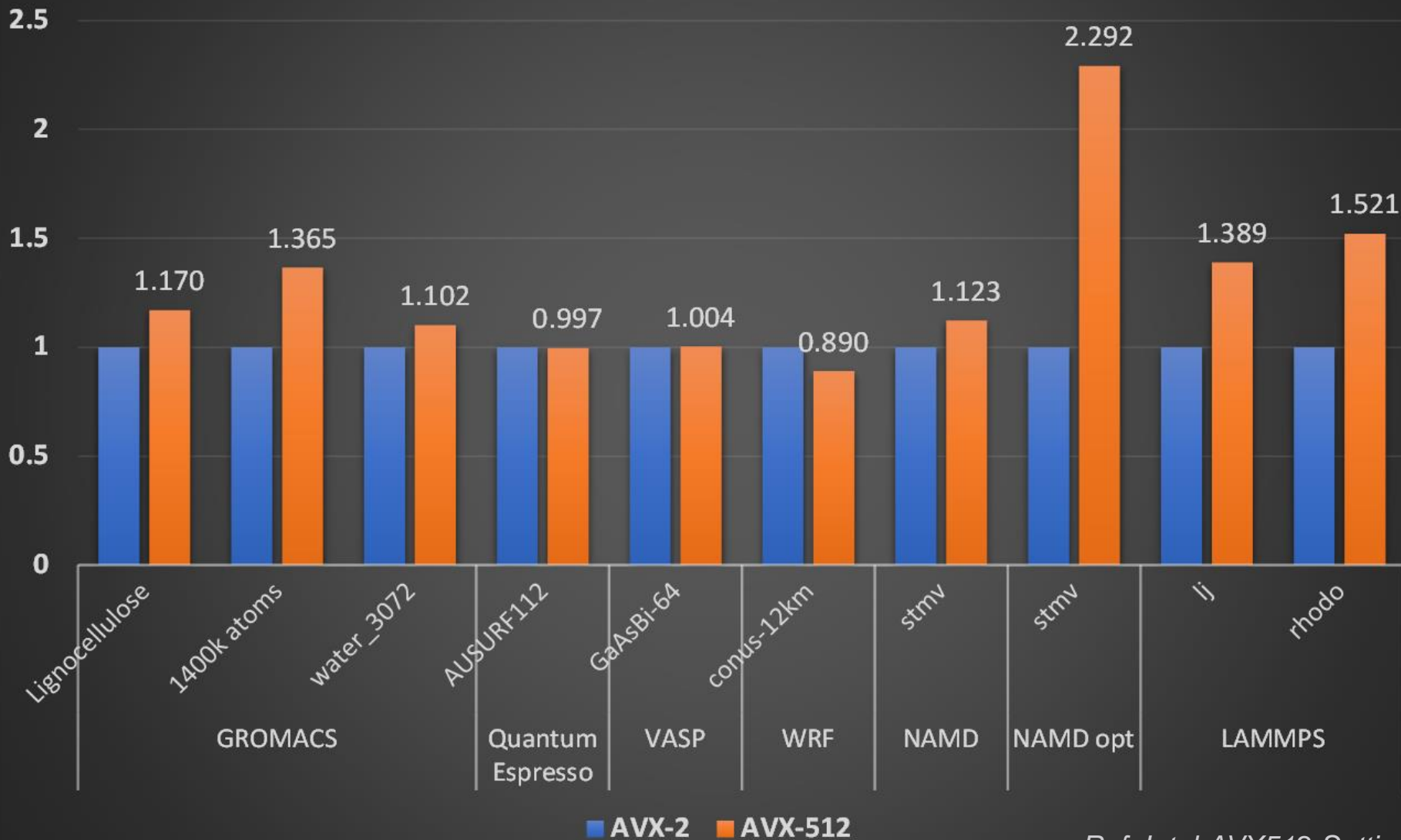
→ HPL (compute bound) is *\*NOT\** a good proxy for scoping job-throughput on realistic workloads.

→ Use memory-bound synthetics: HPCG or STREAM



# ADVANCED VECTOR EXTENSIONS

AVX-512 vs AVX-2 on CLX8280



Some analysis undertaken within Centre of Excellence.

Used Intel system:

- Compiled with AVX2
- Compiled with AVX512

HPL is 'compute bound'

Theoretically;  
 $AVX512 = 2x \text{ AVX2}$

Some improvement over AVX2 ...

... but extra core count on EPYC™ CPUs will make up difference in performance

Ref: Intel-AVX512-Settings

# HPC TOOLS AND RESOURCES

Developer Hub:

<http://developer.amd.com>

- Download compilers, math libraries, uProf profiling tool
- User guides

AMD Tech Docs & White Papers Site:

[https://www.amd.com/en/processors/server-tech-docs/search?f%5B0%5D=product\\_type%3Aepyc\\_7003&f%5B1%5D=server\\_document\\_category%3A14241](https://www.amd.com/en/processors/server-tech-docs/search?f%5B0%5D=product_type%3Aepyc_7003&f%5B1%5D=server_document_category%3A14241)

- Solution Briefs
- Performance Briefs

AMD HPC Tuning Guide for 7003 'Milan' Processors

<https://www.amd.com/system/files/documents/high-performance-computing-tuning-guide-amd-epyc7003-series-processors.pdf>

# TECHNOLOGY FOR THE FUTURE

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**Roadmap for  
Relentless Compute  
Efficiency Gains**

**Aggressive Process &  
Packaging  
Deployment**

**Faster Time to Market  
Through Innovative  
Execution**

**Exascale High-Performance  
Driving Next Wave  
of Innovation**



## CHAR-SUT-01:

|                  |                                 |   |
|------------------|---------------------------------|---|
| System           | Gigabyte MZ62-HD0-00            | <i>For 2<sup>nd</sup> Gen EPYC™ v 3<sup>rd</sup> Gen EPYC™ comparisons, the above System config was used with either a 2<sup>nd</sup> Gen EPYC™ 7742 CPU or 3<sup>rd</sup> Gen EPYC™ 7713/7763 CPU as appropriate</i> |
| BIOS version     | M04 (AGESA 1.0.0.2)             |   |
| Operating System | CentOS 8.3                      | <i>BIOS was set per the HPC Tuning Guide, and altered accordingly for the tests herein</i>  |
| Kernel           | 4.18.0-240.22.1.el8_3.x86_64    |   |
| OFED             | 5.2.2.2                         |   |
| Memory           | 16 channels x DDR4-3200 32GB R2 |   |

---

## CHAR-SUT-02 YYY UPDATE):

|                  |                                 |  |
|------------------|---------------------------------|--|
| System           | 'Daytona'                       | <i>SMT=OFF,, Boost=ON, C2 disabled, Determinism Slider=Power, CPU governor=Performance</i> |
| CPU              | 7742, Rome                      |  |
| BIOS version     | 5.14, 08/15/2019                |  |
| Operating System | CentOS 7.6                      |  |
| Kernel           | 3.10.0-957.10.1.el7.x86_64      |  |
| OFED             | MLNX_OFED_LINUX-4.7-3.2.9.0     |  |
| Memory           | 16 channels x DDR4-3200 32GB R2 |  |

## CHAR-APP-01

### **LAMMPS, 29-OCT-20 Ij**

AOCC+AOCL: -g -O3 -march=znver2 -ffast-math -ffp-contract=fast -DNDEBUG -pthread -fopenmp -std=c++11

### **VASP, 6.1.2 GaAsBi-64** (VASP guide refers to -O2 and not -O3 as default optimisation level)

Intel: -O2 -assume byterecl -w -march=core-avx2 -fma -mavx2 -mfma -free -names lowercase -mkl=sequential -qopenmp -lmkl\_blacs\_openmpi\_lp64 -lmkl\_scalapack\_lp64

### **CP2K, 7.1 H20-256**

AOCC+AOCL compile Line: -O3 -march=znver3 -ffast-math -fopenmp -ffree-form -Hx,47,0x10000008 -Mbackslash

### **Quantum Espresso, 6.5 AUSURF112**

GCC+AOCL compile Line: -O3 -march=znver2 -ffast-math -fopenmp

### **WRF, 3.9.1.1, CONUS 2.5KM**

AOCC: -march=znver3 -ffp-contract=fast -mavx2 -mfma -mprefer-vector-width=256 -Ofast -ffast-math -fopenmp -m64 -w -finline-aggressive -fPIC

### **OpenFOAM, 2012, Motorbike 42m cells**

GCC: -O3 -march=znver2 -mfma -ffp-contract=fast -funroll-loops -fno-signed-zeros -fno-trapping-math -fno-math-errno -ffinite-math-only -fno-rounding-math -fno-signaling-nans -fcx-limited-range -fexcess-precision=fast

### **GROMACS, 2020.4 water\_1536**

AOCC+AOCL: -DGMX\_DOUBLE=0 -O3 -Ofast -g -m64 -march=znver3 -fPIC -ffast-math -ffp-contract=fast -Wno-deprecated-copy -Wno-error=deprecated-copy --gcc-toolchain=/usr -O3 -DNDEBUG -mavx2 -mfma -funroll-all-loops -pthread -fopenmp=libomp

### **NAMD, 2.14**

AOCC+AOCL: -optimize -production -DCMK\_OPTIMIZE -O3 -Ofast -g -m64 -march=znver3 -fPIC -ffp-contract=fast -fopenmp -Wno-deprecated-register -Wno-non-c-typedef-for-linkage -mllvm -inline-threshold=3000 -finline-hint-functions -mllvm -inlinehint-threshold=10000 -finline-functions



## Intel-AVX512-Settings

|                       |   |
|-----------------------|---|
| <b>CPU</b>            | Intel(R) Xeon(R) Platinum 8280 CPU @ 2.70GHz, 28 cores, 2 sockets   |
| <b>Motherboard</b>    | Supermicro X11DPT-B 1.02  |
| <b>Memory</b>         | DDR4 2933MT/s, 376GiB   |
| <b>BIOS</b>           | American Megatrends Inc. v3.1 04/30/2019  |
| <b>Kernel</b>         | 4.18.0-193.el8.x86_64   |
| <b>CPU frequency</b>  | Performance governor, intel_pstate driver, boost active   |
| <b>Hyperthreading</b> | On  |
| <b>Compiler</b>       | ICC/IFORT 19.1.2.254 20200623   |
| <b>Math Library</b>   | Intel MKL 2020.2.254  |
| <b>AVX2 flags</b>     | -O3 -xCORE-AVX2<br>MKL_ENABLE_INSTRUCTIONS=AVX2   |
| <b>AVX512 flags</b>   | -O3 -xCORE-AVX512 -qopt-zmm-usage=high  |
| <b>Codes versions</b> | GROMACS v2021.1<br>Quantum Espresso v6.7<br>VASP v6.2.0<br>WRF v4.2.1<br>NAMD 2.14, NAMD v2.15alpha1<br>LAMMPS stable_29Oct2020 |

# END NOTES

**MLN-073K:** Based on SPECrate®2017\_int\_base on 02/20/2021, a server powered by two 64c AMD EPYC 7763 CPUs has a score of 819 in a compliant result run on an ThinkSystem SR645; with Memory: 2 TB (32 x 64 GB 2Rx4 PC4-3200AA-R), OS: SUSE Linux Enterprise Server 12 SP5 (x86\_64) Kernel 4.12.14-120-default; Compiler: C/C++/Fortran: Version 3.0.0 of AOCC. Versus the current highest score Intel Cascade Lake Refresh server with a score of 397 using 2P Intel Gold 6258R, <https://spec.org/cpu2017/results/res2020q3/cpu2017-20200915-23981.pdf>. SPEC®, SPECrate® and SPEC CPU® are registered trademarks of the Standard Performance Evaluation Corporation. See [www.spec.org](http://www.spec.org) for more information.

**MLN-074K:** Based on SPECrate®2017\_fp\_base on 02/20/2021, a server powered by two 64c AMD EPYC 7763 CPUs has a score of 636 a compliant result run on an ThinkSystem SR665; with Memory: 512 GB (16 x 32 GB 2Rx4 PC4-3200AA-R); OS: Red Hat Enterprise Linux release 8.3 (Ootpa); Compiler: C/C++/Fortran: Version 3.0.0 of AOCC. Versus the current highest score Intel Cascade Lake Refresh server with a score of 309 with a 2P Intel Gold 6258R based server, <https://spec.org/cpu2017/results/res2020q3/cpu2017-20200915-23979.pdf>. SPEC®, SPECrate® and SPEC CPU® are registered trademarks of the Standard Performance Evaluation Corporation. See [www.spec.org](http://www.spec.org) for more information.

**MLN-044A:** SPECjbb®2015-MultiJVM critical-jOPS comparison based on highest system results published as of 03/11/2021. Configurations: 2x AMD EPYC 7763 (301297 SPECjbb2015-MultiJVM critical-jOPS, 359067 SPECjbb2015-MultiJVM max-jOPS, <https://spec.org/jbb2015/results/res2021q1/jbb2015-20210224-00610.html>) versus 2x Intel Xeon Platinum 8280 (138942 SPECjbb2015-MultiJVM critical-jOPS, 169,598 SPECjbb2015-MultiJVM max-jOPS, <https://spec.org/jbb2015/results/res2019q2/jbb2015-20190314-00428.html>) for 117% higher [~2.2x the] performance. SPEC®, and the benchmark SPECjbb® are registered trademarks of the Standard Performance Evaluation Corporation. Learn more at [spec.org](http://spec.org).

**MLN-001:** AMD EPYC™ 7003 Series processors require a BIOS update from your server or motherboard manufacturer if used with a motherboard designed for the AMD EPYC™ 7002 Series processors. A motherboard designed at minimum for EPYC 7002 processors is required for EPYC 7003 Series processors.

**MLN-016:** Results as of 01/28/2021 using SPECrate®2017\_int\_base. The AMD EPYC™ 7763 a measured estimated score of 798 is higher than the current highest 2P server with an AMD EPYC™ 7H12 and a score of 717, <https://spec.org/cpu2017/results/res2020q2/cpu2017-20200525-22554.pdf>. OEM published score(s) for 3rd Gen AMD EPYC™ may vary. SPEC®, SPECrate® and SPEC CPU® are registered trademarks of the Standard Performance Evaluation Corporation. See [www.spec.org](http://www.spec.org) for more information.

**MLN-071K:** Based on SPECrate®2017\_int\_base on 02/20/2021, a server powered by two 64c AMD EPYC 7763 CPUs has a score of 839 which is higher than any currently posted SPEC 2P server score. Per socket score would be  $839/2=419.5$  which is higher than any 1P server score. This is a compliant result run on an ASUS RS720A-E11(KMPP-D32); with Memory: 1 TB (16 x 64 GB 2Rx4 PC4-3200AA-R); OS: SUSE Linux Enterprise Server 15 SP2 (x86\_64) Kernel 5.3.18-22-default; Compiler: C/C++/Fortran: Version 3.0.0 of AOCC. SPEC®, SPECrate® and SPEC CPU® are registered trademarks of the Standard Performance Evaluation Corporation. See [www.spec.org](http://www.spec.org) for more information.

**EPYC-22:** For a complete list of world records see <http://amd.com/worldrecords>.

# END NOTES CONTINUED

**MLN-057K:** Based on SPECrate®2017\_int\_base on 02/20/2021, a server powered by two 8c AMD EPYC™ 72F3 CPU has a measured estimated score of 176 with a per core score of 11.00 which is a higher per core performance score than any currently posted in any SPEC.org publication. SPEC®, SPECrate® and SPEC CPU® are registered trademarks of the Standard Performance Evaluation Corporation. See [www.spec.org](http://www.spec.org) for more information.

**EPYC-22:** For a complete list of world records see <http://amd.com/worldrecords>.

**ROM-693:** 2nd Gen EPYC™ 7H12 powered server with 2 total processors (1-node, 2-socket) scoring 248,942 SPECjbb®2015-MultiJVM critical-jOPS (315,663 max-jOPS, <http://spec.org/jbb2015/results/res2020q2/jbb2015-20200423-00550.html>) has up to 1.79x the SPECjbb® 2015-MultiJVM Critical performance of the highest competitive score of 138942 SPECjbb®2015-MultiJVM critical-jOPS (169598 max-jOPS, <http://www.spec.org/jbb2015/results/res2019q2/jbb2015-20190314-00428.html>) on a Xeon® Platinum 8280 powered server with 2 total processors (1-nodes, 2-socket) as of 6/9/20. SPEC® and SPECjbb® are trademarks of the Standard Performance Evaluation Corporation. See [www.spec.org](http://www.spec.org) for more information.

**CDNA-02:** The AMD Instinct™ MI100 accelerator has 120 compute units (CUs) and 7,680 stream cores at 300W. The Radeon Instinct™ MI50 GPU has 60 CUs and 3,840 stream cores at 300W. CDNA-02

**CDNA-04 :** Calculations by AMD Performance Labs as of Oct 5th, 2020 for the AMD Instinct™ MI100 accelerator designed with AMD CDNA 7nm FinFET process technology at 1,200 MHz peak memory clock resulted in 1.2288 TFLOPS peak theoretical memory bandwidth performance. The results calculated for Radeon Instinct™ MI50 GPU designed with “Vega” 7nm FinFET process technology with 1,000 MHz peak memory clock resulted in 1.024 TFLOPS peak theoretical memory bandwidth performance. CDNA-04

**MI100-04:** Calculations performed by AMD Performance Labs as of Sep 18, 2020 for the AMD Instinct™ MI100 accelerator at 1,502 MHz peak boost engine clock resulted in 184.57 TFLOPS peak theoretical half precision (FP16) and 46.14 TFLOPS peak theoretical single precision (FP32 Matrix) floating-point performance. The results calculated for Radeon Instinct™ MI50 GPU at 1,725 MHz peak engine clock resulted in 26.5 TFLOPS peak theoretical half precision (FP16) and 13.25 TFLOPS peak theoretical single precision (FP32 Matrix) floating-point performance. Server manufacturers may vary configuration offerings yielding different results. MI100-4



# END NOTES CONTINUED

**M100-06:** As of SEP 18th, 2020. AMD Instinct™ MI100 built on AMD CDNA technology accelerators support PCIe® Gen4 providing up to 64 GB/s peak theoretical transport data bandwidth from CPU to GPU per card. Peak theoretical transport rate performance is calculated by Baud Rate \* width in bytes \*# directions = GB/s per card. PCIe Gen4:  $16 * 2 * 2 = 64$  GB/s. AMD Instinct™ MI100 “CDNA” technology-based accelerators include three Infinity Fabric™ link providing up to 276 GB/s peak theoretical GPU to GPU or Peer-to-Peer (P2P) transport rate bandwidth performance per GPU card. Combined with PCIe Gen4 compatibility providing an aggregate GPU card I/O peak bandwidth of up to 340 GB/s. Infinity Fabric link technology peak theoretical transport rate performance is calculated by Baud Rate \* width in bytes \*# directions \*# links = GB/s per card. Infinity Fabric Link:  $23 * 2 * 2 = 92$  GB/s. MI100s have three links:  $92 \text{ GB/s} * 3 \text{ links per GPU} = 276 \text{ GB/s}$ . Four GPU hives provide up to 552 GB/s peak theoretical P2P performance:  $276 \text{ GB/s} * 4 \text{ GPUs} = 1,104 \text{ GB/s}$ , divided by 2 = 552 GB/s. Dual 4 GPU hives in a server provide up to 1.1 TB/s total peak theoretical direct P2P performance per server:  $552 \text{ GB/s per 4 GPU hive} * 2 = 1,104 \text{ GB/s}$ . AMD Infinity Fabric link technology not enabled: Four GPU hives provide up to 256 GB/s peak theoretical P2P performance with PCIe® 4.0:  $64 \text{ GB/s per GPU} * 4 \text{ GPUs} = 256 \text{ GB/s}$ . Radeon Instinct™ MI50 “Vega 7nm” technology-based accelerators support PCIe® Gen 4.0\* providing up to 64 GB/s peak theoretical transport data bandwidth from CPU to GPU per card. Radeon Instinct™ MI50 “Vega 7nm” technology-based accelerators include dual Infinity Fabric™ Links providing up to 184 GB/s peak theoretical GPU to GPU or Peer-to-Peer (P2P) transport rate bandwidth performance per GPU card. Combined with PCIe Gen 4 compatibility providing an aggregate GPU card I/O peak bandwidth of up to 248 GB/s. MI50 based four GPU hives provide up to 368 GB/s peak theoretical P2P performance:  $184 \text{ GB/s} * 4 \text{ GPUs} = 736 \text{ GB/s}$ , divided by 2 = 368 GB/s. Dual 4 GPU hives in a server provide up to 736 GB/s total peak theoretical direct P2P performance per server:  $368 \text{ GB/s per 4 GPU hive} * 2 = 736 \text{ GB/s}$ . Performance guidelines are estimated only and may vary. Refer to server manufacture PCIe Gen4 compatibility and performance guidelines for potential peak performance of the specified server model numbers. Server manufacturers may vary configuration offerings yielding different results. <https://pcisig.com/>, <https://www.chipestimate.com/PCI-Express-Gen-4-a-Big-Pipe-for-Big-Data/Cadence/Technical-Article/2014/04/15>, <https://www.tomshardware.com/news/pcie-4.0-power-speed-express,32525.html> AMD has not independently tested or verified external/third party results/data and bears no responsibility for any errors or omissions therein. MI100-06.

# END NOTES CONTINUED

**MLNTCO-001:** The Bare Metal TCO (total cost of ownership) Estimator solution compares the selected AMD EPYC™ and Intel® Xeon® CPU based server solutions required to deliver a TOTAL\_PERFORMANCE of 25000 unit of integer performance based on published the SPECrate®2017\_int\_base scores for Intel and AMD measured estimated scores for AMD EPYC 7003. This analysis is based on tool VERSION: 02/20/2021 v0.9982. This estimation reflects a 4 year time frame.

This analysis compares a 2 CPU AMD EPYC EPYC\_7763 powered server with a measured estimated SPECrate®2017\_int\_base score of 802; compared to a 2 CPU Intel Xeon Gold\_6258R based server with a SPECrate®2017\_int\_base score of 397, <https://spec.org/cpu2017/results/res2020q3/cpu2017-20200915-23981.pdf>.

Both AMD EPYC and Intel based servers use the same estimated cost for the following elements of the analysis: server chassis size of 2RU at a cost of \$2500 per chassis; internal storage \$380; physical servers managed per admin: 30; fully burdened cost per admin \$110500; server rack size of 42; space allowance per rack of 27 sq feet; monthly cost of data center space \$20 per sq foot; cost per kW for power \$0.12; power drop per rack of 12kW; and a PUE (power usage effectiveness of 2).

The EPYC powered solution estimates are: 32 2P EPYC 7763 powered total servers at a hardware only acquisition cost of \$19232 per server, which includes total system memory of 768GB, which is 6GB of memory / core and a total system memory cost of \$3072; internal storage cost of \$380. The total AMD EPYC hardware acquisition cost for this solution is \$615424. Each server draws ~611kWhr per month. For the 4 years of this EPYC powered solution analysis the: total solution power cost is ~\$225240 which includes the PUE factor; the total admin cost is ~\$471468, and the total real estate cost is ~\$77760. The total 4 year TCO estimate for the AMD solution is \$1389892.

The Intel based solution estimates are: 63 2P Xeon Gold 6258R based total servers at a hardware only acquisition cost of \$12316 per server, which includes total system memory of 384GB, which is 6.9GB of memory / core and a total system memory cost of \$1536; internal storage cost of \$380. The total Intel hardware acquisition cost for this solution is \$775908. Each server draws ~476kWhr per month. For the 4 years of this Intel based solution analysis the: total solution power cost is \$345460 which includes the PUE factor; the total admin cost is ~\$928200, and the total real estate cost is ~\$103680. The total 4 year TCO estimate for the Intel solution is \$2153248.

Delivering 25000 of estimated SPECrate®2017\_int\_base performance, produces the following estimated results: the AMD EPYC solution requires 49% fewer servers  $[1 - (\text{AMD server count} / \text{Intel server count})]$ ; 25% less space  $[1 - (\text{AMD rack count} / \text{Intel rack count})]$ ; 35% less power  $[1 - (\text{AMD power cost} / \text{Intel power cost})]$ ; providing a 35% lower 4 year TCO  $[1 - (\text{AMD TCO} / \text{Intel TCO})]$ .

AMD processor pricing based on 1KU price as of February 2021. Intel® Xeon® Scalable processor data and pricing from <https://ark.intel.com> as of September 2020. All pricing is in USD. Results shown here are estimates and actual results may vary. Product and company names are for informational purposes only and may be trademarks of their respective owners. SPECrate® scores as of 02/20/2021. AMD EPYC performance numbers based on AMD internal estimates and are subject to change based on actual results. SPEC®, SPECrate® and SPEC CPU® are registered trademarks of the Standard Performance Evaluation Corporation. See [www.spec.org](http://www.spec.org) for more information. AMD EPYC performance numbers based on AMD measured internal estimates and are subject to change based on actual results. Results generated by the AMD EPYC™ BARE METAL SERVER TCO ESTIMATION TOOL, VERSION: 02/20/2021 v0.9982.

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